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Scale setting for QCD with $N_f = 3+1$ dynamical quarks

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We present first results of the scale setting for QCD with $N_f = 3+1$ dynamical quarks on the lattice. We use a recently proposed massive renormalization scheme with a non-perturbatively determined clover coefficient. To relate the bare coupling of the simulations to a lattice spacing in fm, we measure t_0^*/a^2, the flow scale t_0 at a mass point with $m_{\text{up}} = m_{\text{down}} = m_{\text{strange}}$ and a physical charm quark mass, and assume that $\sqrt{8t_0^\star} = 0.413(5)(2)\text{fm}$, as determined in [1, 2]. We discuss the setup, tuning procedure, simulation parameters and measurement results for ensembles with three different volumes and present a charmonium spectrum.

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1. Introduction

The omission of a dynamical charm quark from QCD simulations has been shown to have only little effect on low energy observables [3], but can affect quantities with valence charm quarks at a few percent level [4]. Moreover, when the strong coupling is determined on the lattice in $N_\mathrm{f} = 3$ QCD, perturbation theory at the scale of the charm quark is necessary to relate it to the phenomenologically relevant $N_\mathrm{f} = 5$ result. This can introduce an error of up to 1.5% on the Λ parameter [5]. A new action with a novel $O(a)$ improvement scheme, specially tailored towards simulations including a charm quark, has been proposed in [6]. We report on first large volume simulations using this action, and in particular concentrate on setting the scale.

The goal is to map out the relation between the bare coupling g_0 and the lattice spacing a in fm. This relation is, up to lattice artifacts, independent of the quark masses. The standard procedure is to determine an experimentally accessible dimensionful quantity at the physical mass point in lattice units, and obtain the lattice spacing by using the experimental input. This usually requires simulations of whole chiral trajectories at each lattice spacing. We propose a method for scale setting that is orders of magnitude cheaper and requires only simulations at the flavor $SU(3)$ symmetric point, where the three light quark masses are equal and

$$\phi_4 \equiv 8t_0\left(m_\mathrm{K}^2 + \frac{m_\pi^2}{2}\right) = 12t_0 m_{\pi,\mathrm{K}}^2 = 1.11\,, \tag{1.1}$$

$$\phi_5 \equiv \sqrt{8t_0}\,(m_{\mathrm{D_s}} + 2m_\mathrm{D}) = \sqrt{72t_0}\,m_{\mathrm{D,D_s}} = 11.94\,, \tag{1.2}$$

At this mass point $\sqrt{8t_0^\star} = 0.413(5)(2)$fm has been determined in [1, 2]. Due to decoupling it has the same value in the $3+1$ flavor theory up to a couple per mille, as long as the fourth quark's mass is at least as heavy as a charm quark, but this is what is enforced by the second condition Eq. 1.2.

Once the relation between g_0 and a is mapped out on this particular mass point, one can proceed constructing chiral trajectories, *e.g.*, along lines where ϕ_4 and ϕ_5 are constant. But already the $SU(3)$ symmetric ensembles are highly useful. They can be the starting point for the determination of fundamental parameters of QCD, but also can be used directly for charm physics, where the unphysical light quark masses play only a small role.

2. Simulation setup and scale setting

Renormalization and improvement conditions are imposed at zero quark mass in non-perturbative mass-independent schemes. This has many advantages. Z-factors and improvement coefficients depend only on the bare coupling and renormalization scale, and some perturbative coefficients, like b_0 and b_1 in the expansion of the beta-function, are scheme independent. The drawback however is, that the $O(a)$ improvement pattern with Wilson fermions can become very complicated. For example, the renormalized $O(a)$ improved quark mass is given by [6]

$$\begin{aligned} m_{\mathrm{R},i} = Z_m(\tilde{g}_0^2, a\mu)\Big[& m_{\mathrm{q},i} + \left(r_m(\tilde{g}_0^2) - 1\right)\frac{\mathrm{tr}\,[M_\mathrm{q}]}{N_\mathrm{f}} + a\Big\{ b_m(g_0^2)m_{\mathrm{q},i}^2 + \bar{b}_m(g_0^2)\,\mathrm{tr}\,[M_\mathrm{q}]\,m_{\mathrm{q},i} \\ & + \left(r_m(g_0^2)d_m(g_0^2) - b_m(g_0^2)\right)\frac{\mathrm{tr}\,[M_\mathrm{q}^2]}{N_\mathrm{f}} + \left(r_m(g_0^2)\bar{d}_m(g_0^2) - \bar{b}_m(g_0^2)\right)\frac{\left(\mathrm{tr}\,[M_\mathrm{q}]\right)^2}{N_\mathrm{f}}\Big\}\Big]\,, \end{aligned} \tag{2.1}$$

$$\tilde{g}_0^2 = g_0^2\left(1 + ab_\mathrm{g}(g_0^2)\,\mathrm{tr}\,[M_\mathrm{q}]/N_\mathrm{f}\right).$$

Most of the improvement coefficients (b_m, etc.) are not known beyond 1-loop of perturbation theory. This can lead to large uncanceled $O(a)$ effects, if $a\,\mathrm{tr}\,(M_q)$ or $am_{\mathrm{q},i}$ are large. To avoid this complicated improvement pattern, one can give up the mass-independence of the scheme. This allows to absorb all b and d terms into the definition of the, now mass dependent, renormalization factors. A scheme to do so was proposed in [6] and the mass dependent clover coefficient c_{sw} in the clover action term $S_{\mathrm{SW}} = a^5 c_{\mathrm{sw}}(g_0^2, M_{\mathrm{q}}) \sum_x \bar{\psi}(x) \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x) \psi(x)$ has been determined non-perturbatively. We apply this action for the first time to large volume simulations with a physical charm quark mass. For a first estimate of the bare coupling and quark masses we use the tuning results in [6], determined on a line of constant physics (LCP). For our first simulation we choose a bare coupling $\beta = 3.24$, light quark masses given by $\kappa_{u,d,s} = 0.134484$ and a charm quark mass by $\kappa_c = 0.12$. For the algorithmic parameters, we started with the setup of CLS's H400 simulation, cf. [7], to which we added the charm quark. The new contribution to the action was not further factorized and the corresponding forces were integrated on the second level of our three level integrator. For our simulations we use openQCD version 1.6[1] [8] with open boundary conditions in time direction and twisted-mass reweighting, 2nd and 4th order OMF integrators [9], SAP preconditioning and low-mode-deflation based on local coherence [10, 11]. For a full specification of the action with open boundary conditions we also need $c_0 = 5/3$ for the Lüscher–Weisz action, boundary improvement coefficients $c_F = c_G = 1.0$ and the clover coefficient from the fit formula [6]

$$c_{\mathrm{sw}}(g_0^2 = 6/3.24) = \frac{1 + Ag_0^2 + Bg_0^4}{1 + (A - 0.196)g_0^2} = 2.18859\,, \quad A = -0.257\,, \quad B = -0.050\,.$$

The u/d quark doublet is simulated with a weight proportional to $\det[(D_{oo})^2] \frac{\det[\hat{D}^\dagger \hat{D} + \mu^2]^2}{\det[\hat{D}^\dagger \hat{D} + 2\cdot\mu^2]}$ in terms of the even–odd preconditioned Dirac operator $\hat{D}$. The strange and charm quarks are simulated with RHMC, and the two rational functions have degrees 12 and 10, respectively with ranges optimized during the tuning process. Both the doublet and the rational parts need reweighting and are further factorized according to [12]

$$\det[\hat{D}^2 + \mu^2] = \det[\hat{D}^\dagger \hat{D} + \mu_0^2] \times \frac{\det[\hat{D}^\dagger \hat{D} + \mu_1^2]}{\det[\hat{D}^\dagger \hat{D} + \mu_0^2]} \times \ldots \times \frac{\det[\hat{D}^\dagger \hat{D} + \mu^2]}{\det[\hat{D}^\dagger \hat{D} + \mu_N^2]},$$

such that we have 13 pseudo-fermion fields and 14 actions in total.

After thermalization on spatially smaller lattices and subsequent doubling of the spatial dimensions, flow observables and meson masses were computed on a more-or-less thermalized subset of configurations. It turned out that the desired tuning point was missed by quite a bit. What makes the tuning process non-trivial is the fact that in ϕ_4 and ϕ_5 the mass dependence of t_0 and the meson masses go in opposite directions. The final tuning point turns out to be

$$\kappa_{u,d,s} = 0.13440733, \quad \kappa_c = 0.12784.$$

With these final parameters we produced two high statistics ensembles A1 and A2 with two different lattice sizes given in Table 1 and a short ensemble A0 on a smaller lattice to study finite size effects. A computation of $t_0^\star/a^2$ on these ensembles, together with the known value of $\sqrt{8t_0^\star} = 0.413(5)(2)$fm [1, 2], yields values for the lattice spacings in fm. A setup with open boundaries in

[1] M. Lüscher, S. Schaefer, `http://luscher.web.cern.ch/luscher/openQCD/`

the temporal direction and periodic boundaries in spatial directions allows us to reach fine lattice spacings [13], which is crucial for simulations with a dynamical charm quark in the sea. The measurements of the mesonic two-point functions were carried out with the open-source (GPL v2) program “mesons" [2], the degenerate pion/kaon and D-/D_s-meson masses in lattice units as well as our final tuning parameters are also shown in Table 1. The results of flow measurements and topological charges are presented in Table 2. The integrated autocorrelation time of t_0 is $\tau_{\text{int},t_0} \approx 20 \pm 10$ [4 MDU]. Assuming decoupling, *i*.e., $t_0^{\star}|_{N_f=3+1} = t_0^{\star}|_{N_f=3} + O(1/m^2_{\text{charm}})$, our value of $t_0/a^2 \approx 7.4$ corresponds to a lattice spacing $a \approx 0.054$ fm. The physical size of our $L/a = 32$ lattice is $L \approx 1.73$ fm with $m_\pi L = 3.5$, which is a bit small, but finite size effects seem to be under control, as the comparison with $L/a = 48$ shows. Fig. 1 presents example histories of the action density of the flowed gauge field and the topological charge.

ens.	$\frac{T}{a} \times \frac{L^3}{a^3}$	$Lm_\pi^\star$	N_{traj} (MDUs)	$am_{\pi,K}$	am_{D,D_s}	ϕ_4	ϕ_5
A0	96×16^3	1.75	1400 (3800)	0.310(6)	0.614(17)	10.22(90)	15.48(43)
A1	96×32^3	3.5	3908 (7816)	0.1137(8)	0.5247(7)	1.159(17)	12.168(40)
A2	128×48^3	5.3	3868 (7736)	0.1107(3)	0.5228(4)	1.087(6)	12.059(20)

Table 1: Lattice sizes, statistics and tuning results of the three ensembles with bare coupling $\beta = 3.24$ corresponding to $a = 0.054$fm, and quark masses $\kappa_{u,d,s} = 0.13440733$ and $\kappa_c = 0.12784$.

ens.	N_{ms}	t_0/a^2	τ_{int,t_0}	t_c/a^2	τ_{int,t_c}	w_0^2/a^2	τ_{int,w_0}	Q^2	τ_{int,Q^2}
A0	700	8.83(23)	10(2)	4.12(9)	9(4)	-	-	0.83(11)	6(1)
A1	1954	7.43(4)	16(7)	3.88(1)	11(4)	10.26(13)	24(12)	1.08(4)	5(1)
A2	1934	7.36(3)	27(15)	3.86(1)	19(12)	10.13(8)	30(17)	6.60(19)	5(2)

Table 2: Flow measurement results and topological charge with integrated autocorrelation times.

3. Charmonium spectrum and finite size effects

In figure 2 we show the meson spectrum of our ensemble A2. We get a very clear signal up to the J/Ψ state and can extract reasonable plateau values for higher charmonium states summarized in table 3. We find good agreement for charmonia with PDG data because they contain only charm valence quarks which in our simulations have their physical mass value. Further, the sum of the degenerate light quark masses is at its physical value and since there are no light quarks in the valence sector, the derivatives of the charmonium masses with respect to light quark masses are equal, *i.e.* $dm_x/dm_{\text{up}} = dm_x/dm_{\text{down}} = dm_x/dm_{\text{strange}}$. If we want to correct the degenerate light quark masses to their physical values via $m_x^{\text{phys}} = m_x + (\Delta_{\text{up}} + \Delta_{\text{down}} + \Delta_{\text{strange}})\frac{dm_x}{dm_u} + \text{O}(\Delta^2)$, it is clear that the linear term vanishes, because ϕ_4 is chosen such that $\Delta_{\text{up}} = \Delta_{\text{down}} = -0.5\Delta_{\text{strange}}$ ($m_{u,d,s} = \sum_{i=u,d,s} m_i^{\text{phys}}/3$) and we only have $\text{O}(\Delta^2)$ corrections.

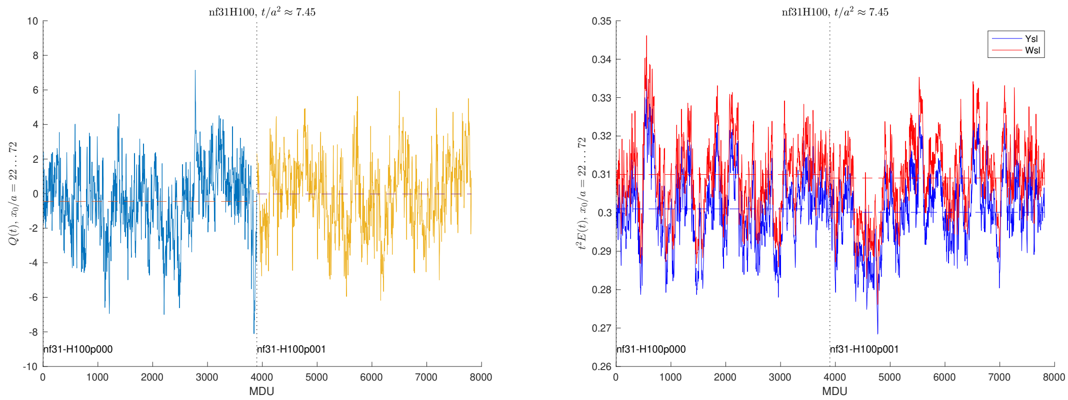

Figure 1: Histories of the topological charge $Q(t)$ (left) and of $t^2E(t)$ (right) where $E(t) = \frac{1}{4}G^a_{\mu\nu}(t)G^a_{\mu\nu}(t)$ is the action density of the flowed gauge field, where t corresponds approximately to t_0. The two curves show the results for different discretizations of $E(t)$, symmetric (blue) and plaquette (red), which differ by $O(a^2)$ effects. Both replica of ensemble A1 are shown, due to open boundary conditions we average only over time slices $x_0/a = 22\ldots72$, as indicated on the ordinate.

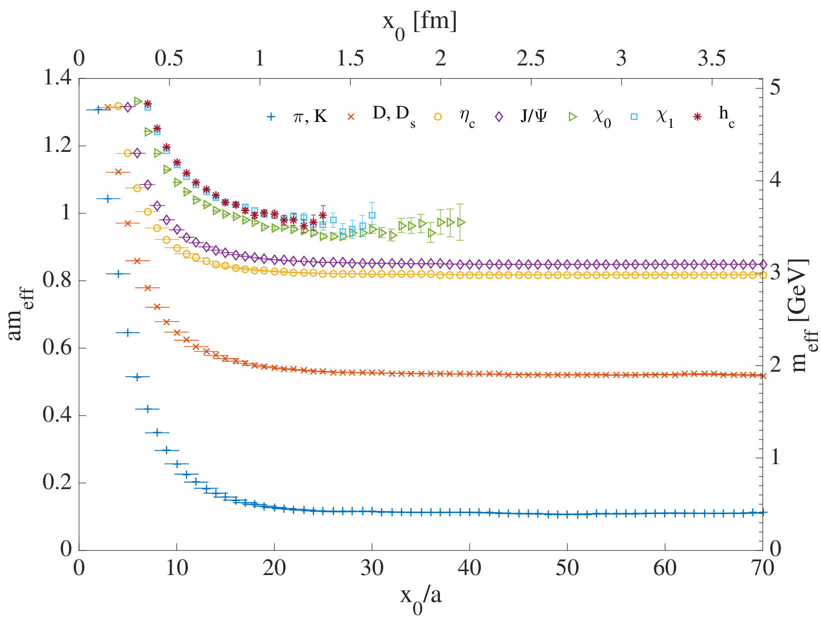

Figure 2: Effective masses of the pion/kaon, D- and D_s-meson, charmonium states η_c, J/Ψ, χ_0, χ_1 and h_c (from bottom to top).

Next, we study finite volume effects of am_π following [14, 15], who propose an analytic scaling formula from chiral perturbation theory in the p-expansion

$$m_\pi(L) = m_\pi\left[1 + \frac{\xi_\pi \tilde{g}_1(Lm_\pi)}{2N_\mathrm{f}} + \mathscr{O}(\xi_\pi^2)\right],\ \tilde{g}_1(x) = \sum_{n=1}^{\infty}\frac{4m(n)}{\sqrt{n}x}K_1(\sqrt{n}x),\ \xi_\pi = \frac{m_\pi^2}{(4\pi F_\pi)^2}. \tag{3.1}$$

[2]T. Korzec, `https://github.com/to-ko/mesons`

The analytic χPT prediction together with our lattice data is presented in Fig. 3, for the pion mass and decay constant at the SU(3) flavor symmetrical point we take the values determined on the finest lattice in [2]. In the range of pion masses and volumes considered the agreement between the one-loop analytical prediction and our lattice data is poor, especially for $Lm_\pi < 3.5$.

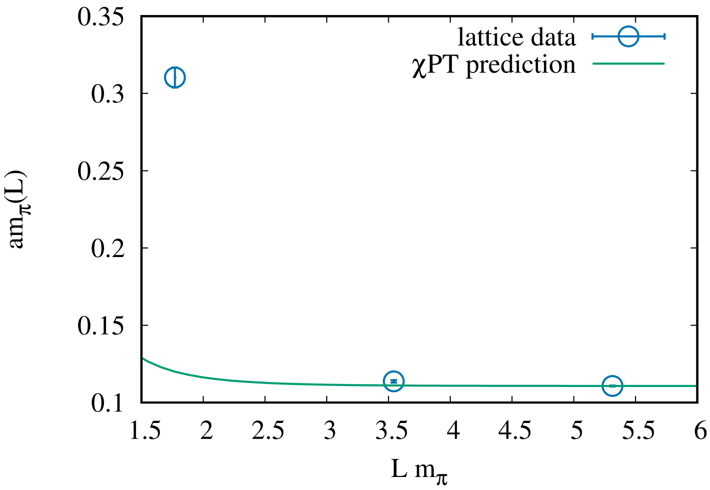

Figure 3: Finite volume scaling effect of am_π with χPT formula in Eq. 3.1 from [14, 15]

4. Conclusions & Outlook

We presented the scale setting and tuning of $N_\mathrm{f} = 3+1$ QCD using a massive renormalization scheme with a non-perturbatively determined clover coefficient from [6]. We produced two ensembles with lattice sizes 96×32^3 and 128×48^3 and determine the lattice spacing $a = 0.054$ fm. As a first physics result, we measure the masses of the charmonium states η_c, J/ψ, χ_{c0}, χ_{c_1} and h_c, which we find close to their PDG values. We further plan to study decoupling of the charm quark with light quarks on our ensembles, measure the charmonium sigma terms, disconnected quark loop contributions and the strong coupling α_S. To approach the continuum limit we need even larger and finer ensembles. The tuning of ensemble B on a 144×48^3 lattice at finer lattice spacing ($a \approx 0.043$fm) is finished and production started, and a final ensemble C on a 192×64^3 at an even finer lattice spacing may also be simulated.

	η_c	J/ψ	χ_{c0}	χ_{c_1}	h_c
am_{eff}	0.8180(2)	0.8489(2)	0.9398(86)	0.9833(72)	0.9902(81)
m_{eff} [GeV]	2.9890(7)	3.1019(7)	3.434(31)	3.593(26)	3.618(30)
PDG [GeV]	2.9834(5)	3.096900(6)	3.4148(3)	3.51066(7)	3.52538(11)

Table 3: Effective masses of charmonium states together with their PDG values.

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